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Oscillation of the Radial Distribution Function

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We prove that the radial distribution function oscillates at low density in a system with a short-range nonnegative potential and investigate the branching of the solutions of an approximate equation of state.

KEY WORDS: Nonnegative operator; hard-sphere model; radial distribution function; equation of state.

1. INTRODUCTION

Gonchar[(1–4)] has proposed a new set of strict equations for correlation functions of equilibrium classical statistical mechanics. The solution was constructed for the pair repulsive interaction potential at arbitrary values of activity z and temperature with the help of some nonlinear monotonically increasing map L. The work in refs. 1–3 generalized the well-known fundamental results of refs. 5–8. In specific physical applications it is important to have approximate equations for some quantities from which correlation functions and the equation of state may easily be obtained. One possible way was analyzed in ref. 4 and investigated for the simplest case in refs. 9 and 10. We prove that oscillations of a radial distribution function appear in systems with a short-range interaction at arbitrary low density and investigate the branching of the solution of the approximate equation of state.

We use the notation introduced in refs. 1–4:

$$\{t, X\}_n = \{\{t_1, x_1\},\dots, \{t_n, x_n\}\}, \qquad 0 \leqslant t_j \leqslant 1, \qquad x_j \in V \subset R^\nu$$

$$B_1 = \{F = \{f_1(\{t, X\}_1),\dots, f_n(\{t, X\}_n),\dots\}:$$

$$|F|_1 = \sup_n \operatorname*{essup}_{\{t, X\}_n \in [[0,1] * V]^n} |f_n(\{t, X\}_n)| < +\infty\}$$

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where f_n is a measurable function on $\Gamma_n = [[0, 1] * V]^n$,

$$\rho_0 = \{1, 0, 0, 0,...\}, \qquad \theta = \{0, 0, 0, 0,...\}, \qquad \bar{e} = \{1, 1, 1, 1,...\}$$

Define operators T and K for a set of nonnegative kernels $K_n(\{t, X\}_n; \{s, y\})$ and measure $d\mu(s)$ satisfying the conditions

$$\int_0^1 d\mu(s) < +\infty$$

$$b_0 = \sup_{\{t,X\}_n} \int_0^1 d\mu(s) \int_V dy\, K_n(\{t, X\}_n; \{s, y\}) < +\infty:$$

$$TF = \{0, f_1(\{t, X\}_1), f_2(\{t, X\}_2),...\}$$

$$KF = \{(KF)_n(\{t, X\}_n)\}_{n=1,+\infty}$$

where

$$(KF)_n(\{t, X\}_n)$$
$$= \int_0^{t_n} dt'_n \int_0^1 d\mu(s) \int_V dy\, K_n(\{t, X\}'_n; \leqslant s, y\})\, f_{n+1}(\{t, X\}'_n, \{s, y\})$$

$$\{t, X\}'_n = \{\{t_1, x_1\},..., \{t_{n-1}, x_{n-1}\}, \{t'_n, x_n\}\}$$

Define a nonlinear operator L on B_1:

$$L(F) = \{L_n(F)(\{t, X\}_n)\}_{n=1,+\infty}$$

for

$$L_n(F)(\{t, X\}_n)$$
$$= \exp\left\{-z \int_0^{t_n} dt'_n \int_0^1 d\mu(s) \int_V dy\, K_n(\{t, X\}'_n; \{s, y\})\right.$$
$$\times \exp\left[-z \int_0^s ds' \int_0^1 d\mu(s_1) \int_V dy_1\, K_{n+1}(\{t, X\}'_n, \{s', y\}; \{s_1, y_1\})\right.$$
$$\left.\left.\times f_{n+2}(\{t, X\}'_n, \{s', y\}, \{s_1, y_1\})\right]\right\}$$

and denote the nth iteration of L at F as $L^n(F)$. Obviously there exist limits

$$\lim_{n \to +\infty} L^n(\theta) = L^\infty(\theta), \qquad \lim_{n \to +\infty} L^n(\bar{e}) = L^\infty(\bar{e})$$

such that $\theta \leqslant L^\infty(\theta) \leqslant L^\infty(\bar{e}) \leqslant \bar{e}$.

The equation

$$\rho = T\rho - zK\rho + \rho_0 \tag{1}$$

possesses a positive solution in B_1 for arbitrary $z > 0$,[4]

$$\rho_n(\{t, X\}_n) = \prod_{l=1}^{k} H_{2l-1}(\{t, X\}_{2l-1}) \prod_{l=1}^{m} \exp[-z(KH)_{2l}(\{t, X\}_{2l})] \tag{2}$$

where $m = k$, for $n = 2k$ and $m = k - 1$ for $n = 2k - 1$,

$$H = L(H) \tag{3}$$

Now we fix $d\mu(s) = \delta(s-1)\, ds$ and define

$$\chi_\beta(x-y) = 1 - e^{-\beta U(x-y)}$$

for the pair repulsive potential $U(x-y)$, supposing

$$\chi_\beta|_{\text{int supp } U} > 0, \qquad C(\beta) = \int_{R^\nu} \chi_\beta(x)\, dx < +\infty$$

Here $\beta = 1/k_B T$ is the inverse temperature, and $V = R^\nu$ is the coordinate space of the physical system. The correlation functions of classical statistical mechanics can be expressed in terms of the solution (1):

$$g_n(x_1,..., x_n) = z^n \exp\left[-\beta \sum_{i<j} U(x_i - x_j)\right] \rho_n(\{1, x_1\},..., \{1, x_n\})$$

for

$$K_n(\{t, X\}_n; \{s, y\}) = \chi_\beta(x_n - y) \prod_{j=1}^{n-1} [1 - t_j \chi_\beta(x_j - y)] \tag{4}$$

we write expresions for the density

$$\rho(z) = zH_1(\{1, x\}) \tag{5}$$

and the radial distribution function

$$G(x_1, x_2) = \exp[-\beta U(x_1 - x_2)]\, H_2(\{1, x_1\}, \{1, x_2\})/H_1(\{1, x_1\}) \tag{6}$$

for Eq. (3) possessing a unique solution H for which

$$H_n = L_n(H) = \exp[-z(KH)_n]$$

See ref. 4, Eq. (1.3.11), Proposition 1.3.4, and Theorem 1.4.5.

2. OSCILLATIONS OF THE RADIAL DISTRIBUTION FUNCTION AT LOW DENSITY IN A SYSTEM WITH A SHORT-RANGE INTERACTION

The solution of Eq. (3) can be expressed in terms of a signature-changing variety (for small values of z)

$$\ln[H_n(\{t, X\}_n)] = \sum_{j=1}^{+\infty} f_n(j)(\{t, X\}_n)(-z)^j \tag{7}$$

where

$$f_n(j+1)(\{t, X\}_n) = \int_0^{t_n} dt'_n \int_V dy\, K_n(\{t, X\}'_n; \{1, y\}) \times \sum_{|\sum_{k=1, j(k)\geq 0}^{+\infty} kj(k) = j|} \prod_{k=1}^{j} [f_{n+1}^{j(k)}(k)(\{t, X\}'_n, \{1, y\})/j(k)!] \tag{8}$$

Here the addition of products is performed over all sequences of integer nonnegative numbers $\{j(k)\}$ satisfying the condition written out in the brackets under the first addition sign. We consider the kernels

$$K_n^N(\{t, X\}_n; \{s, y\}) = \chi_\beta(x_n - y) \sum_{j=\max(1, n-N+1)}^{n-1} [1 - t_j \chi_\beta(x_j - y)]$$

for $V = R^\nu$, diam supp $U = 2\sigma$. The case $N = +\infty$ corresponds to an exact equation of state (1)–(5); the case $N < +\infty$ corresponds to an approximation up to the $(N+1)$-th virial coefficient with a further reduction to a nonlinear equation for some function with a finite number of variables; see Section 2.5.[4] We use the notation $G_N(x_1, x_2)$ for the approximate radial distribution function (6) calculated for the approximate equation of state (1)–(3, 5) with K_n^N instead of K_n.

Lemma 1. $f_n(j)(\{t, X\}_n)$ does not depend on $\{t, X\}_{n-N}$ for $n > N$.

Proof. We use induction (on j). In accordance with (8),

$$f_n(1)(\{t, X\}_n) = \int_0^{t_n} dt'_n \int_{R^\nu} dy\, \chi_\beta(x_n - y) \prod_{l=\max(1, n-N+1)}^{n-1} [1 - t_l \chi_\beta(x_l - y)] \tag{9}$$

There are multipliers $[1 - t_l \chi_\beta(x_l - y)]$ for $l = n - N + 1, \ldots, n-1$ only in the integrand (9); thus the statement of the lemma is true for $j = 1$. Let the proposition of the lemma be valid for natural j from 1 to J and all natural $n > N$ and its condition be valid for $j = J + 1$. We have

$$f_n(J+1)(\{t, X\}_n)$$
$$= \int_0^{t_n} dt'_n \int_{R^\nu} dy\, \chi_\beta(x_n - y) \prod_{l=\max(1, n-N+1)}^{n-1} [1 - t_l \chi_\beta(x_l - y)]$$
$$\times \sum_{|\sum_{k=1, j(k)\geq 0}^{J} kj(k) = J|} \prod_{k=1}^{J} [f_{n+1}^{j(k)}(k)(\{t, X\}'_n, \{1, y\})/j(k)!] \quad (10)$$

$f_{n+1}(k)(\{t, X\}_{n+1})$ does not depend on $\{t, X\}_{n-N+1}$ and there are multipliers $[1 - t_l \chi_\beta(x_l - y)]$ for $l = n - N + 1, \ldots, n - 1$ only in the integrand (10). Thus the lemma has been proved by induction.

Lemma 2. $f_n(j)(\{t, X\}_n)$ does not depend on $\{t_1, x_1\}$ for arbitrary natural j, n, and any $\{t, X\}_n$ such that:

(i) $2 \leqslant n \leqslant N$.

(ii) $|x_l - x_{l+1}| \leqslant \sigma$ for $l = 2, \ldots, n-1$.

(iii) $|x_1 - x_2| > \min(N, j + n - 1)\sigma$.

Proof. If the condition of the lemma is valid, then

$$\begin{aligned} \chi_\beta(x_n - y) \neq 0 &\Rightarrow |x_n - y| \leqslant \sigma \\ &\Rightarrow |x_1 - y| \geqslant |x_1 - x_2| - |x_2 - x_3| - \cdots - |x_n - y| \\ &> \min(N - n + 1, j)\sigma \\ &\Rightarrow \chi_\beta(x_1 - y) = 0 \end{aligned}$$

in expressions (9)–(10). One should use induction (on j) in order to end the proof (with the help of lemma 1 for $N < +\infty$).

The value of $f_n(j)(\{t, X\}_n)$ does not increase for increasing t_1 due to the recurrence relations (9)–(10). The previous lemmas state the sufficient conditions for the value $f_n(j)(\{t, X\}_n)$ to be independent of t_1.

Lemma 3. We have

$$f_2(j)(\{t'_1, x_1\}\{1, x_2\}) - f_2(j)(\{t''_1, x_1\}\{1, x_2\}) > 0$$

if $0 \leqslant t'_1 < t''_1 \leqslant 1$ and $0 < |x_1 - x_2| < \min(N, j+1)\sigma$.

Proof. We have

$$(K^j\bar{e})_n(\{t, X\}_{n-1}, \{1, x_n\})$$
$$= \int_0^1 dt_n \int_{R^\nu} dx_{n+1} \cdots \int_0^1 dt_{n+j} \int_{R^\nu} dx_{n+j+1}$$
$$\times \prod_{k=1}^{j} \left\{ \chi_\beta(x_{n+k} - x_{n+k+1}) \prod_{l=\max(1,n+k-N)}^{n+k-1} [1 - t_l \chi_\beta(x_l - x_{n+k+1})] \right\} \geqslant 0$$

for arbitrary natural j and n. Furthermore, the integrand is positive for almost all t_k (being from $[0, 1)$, $k = 1, 2,..., n+j$, and x_{n+k+1} such that $|x_{n+k+1} - x_n| < \sigma/2$, which implies

$$|x_{n+k+1} - x_{n+k}| < \sigma \Rightarrow \chi_\beta(x_{n+k+1} - x_{n+k}) > 0 \qquad \text{for} \quad k = 1, 2,..., j$$

Thus $(K^j\bar{e})_n(\{t, X\}_{n-1}, \{1, x_n\})$ is positive for arbitrary natural j and n if $t_k < 1$ for $k < n$.

Now, $f_2(j)(\{t_1, x_1\}, \{1, x_2\})$ equals the sum of $(K^j\bar{e})_2(\{t_1, x_1\}, \{1, x_2\})$ and terms not increasing for increasing t_1 [see Eqs. (8)–(10)]. Denote $N' = \min(N, j+1)$. Then

$$(K^j\bar{e})_2(\{t_1, x_1\}, \{1, x_2\})$$
$$= \prod_{k=2}^{N'} \left\{ \int_0^1 dt_k \int_{R^\nu} dx_{k+1}\, \chi_\beta(x_k - x_{k+1}) \prod_{l=1}^{k-1} [1 - t_l \chi_\beta(x_l - x_{k+1})] \right\}$$
$$\times (K^{j-N'+1}\bar{e})_{N'+1}(\{t, X\}_{N'}, \{1, x_{N'+1}\})$$

We have

$$(K^{j-N'+1}\bar{e})_{N'+1}(\{t, X\}_{N'}, \{1, x_{N'+1}\}) = 1 \qquad \text{for} \quad N' = j+1$$

It is positive for $t_2, t_3,..., t_{N'}$ being from $(0, 1)$ and does not depend on t_1, x_1 for $N' = N$ (see expression for K_n^N). Let the real, positive number d be less than $\sigma N'/|x_1 - x_2| - 1$ and x_k be a point of R^ν such that

$$|x_k - x_2 - (k-2)(x_1 - x_2)/N'| < |x_1 - x_2|\, d/2N' \qquad \text{for} \quad k = 3, 4,..., N'+1$$

Then

$$\begin{aligned} |x_k - x_{k+1}| &\leqslant |x_k - x_2 - (k-2)(x_1 - x_2)/N'| \\ &\quad + |x_{k+1} - x_2 - (k-1)(x_1 - x_2)/N'| + |x_1 - x_2|/N' \\ &< (d/2 + d/2 + 1)\,|x_1 - x_2|/N' \\ &= (d+1)\,|x_1 - x_2|/N' < \sigma \end{aligned}$$

which implies the inequality $\chi_\beta(x_k - x_{k+1}) > 0$ for $k = 2, 3,..., N'$.

Thus we have pointed out a domain of values $t_2,\ldots, t_{N'}$ and $x_3, x_4,\ldots, x_{N'+1}$ for which the integrand of the expression obtained above for $(K^j\bar{e})_2(\{t_1, x_1\}, \{1, x_2\})$ (being nonnegative in any case) is positive for $t_1 < 1$. The following inequalities are valid for these values of $t_2,\ldots, t_{N'}$ and $x_3, x_4,\ldots, x_{N'+1}$:

$$\begin{aligned} |x_1 - x_{N'+1}| &\leqslant |x_1 - x_2 - (N'-1)(x_1 - x_2)/N'| \\ &\qquad + |x_{N'+1} - x_2 - (N'-1)(x_1 - x_2)/N'| \\ &< (1 + d/2)\,|x_1 - x_2|/N' < \sigma \\ &\Rightarrow \chi_\beta(x_1 - x_{N'+1}) > 0 \end{aligned}$$

The difference

$$\begin{aligned} &(K^j\bar{e})_2(\{t_1', x_1\}, \{1, x_2\}) - (K^j\bar{e})_2(\{t_1'', x_1\}, \{1, x_2\}) \\ &= \int_0^1 dt_2 \int dx_3 \cdots \int_0^1 dt_{N'} \int dx_{N'+1}\, (K^{j-N'+1}\bar{e})_{N'+1}(\{t, X\}_{N'}, \{1, x_{N'+1}\}) \\ &\quad \times \prod_{k=2}^{N'} \left\{ \chi_\beta(x_k - x_{k+1}) \prod_{l=2}^{k-1} [1 - t_l \chi_\beta(x_l - x_{k+1})] \right\} \\ &\quad \times \left\{ \prod_{k=2}^{N'} [1 - t_1' \chi_\beta(x_1 - x_{k+1})] - \prod_{k=2}^{N'} [1 - t_1'' \chi_\beta(x_1 - x_{k+1})] \right\} \end{aligned}$$

is positive for $0 \leqslant t_1' < t_1'' \leqslant 1$ iff there exists a domain of values of $t_2,\ldots, t_{N'}$ and $x_3,\ldots, x_{N'+1}$ such that the difference $\{\cdots\}$ is positive with other multipliers of the integrand. But we have pointed out this domain (above), for which the following inequalities are valid:

$$1 - t_1' \chi_\beta(x_1 - x_{k+1}) \geqslant 1 - t_1'' \chi_\beta(x_1 - x_{k+1}) \geqslant 0, \qquad k = 2,\ldots, N'-1$$

(the left part of this inequality is positive for $t_1' < 1$);

$$1 - t_1' \chi_\beta(x_1 - x_{N'+1}) > 1 - t_1'' \chi_\beta(x_1 - x_{N'+1}) \geqslant 0$$

Let $\hat{f}_1 = C(\beta)$,

$$\hat{f}_{J+1} = C(\beta) \sum_{|\sum_{k=1,\, j(k)\geqslant 0}^{J} kj(k) = J|} \prod_{k=1}^{J} [\hat{f}_k^{j(k)}/j(k)!] \qquad \text{for} \quad J \geqslant 1$$

The equation

$$\hat{f} = zC(\beta)\, e^{\hat{f}}$$

possesses solution

$$\hat{f} = \sum_{j=1}^{+\infty} \hat{f}_j z^j$$

for $|z| \leqslant 1/eC(\beta)$. It is easy to prove that $f_n(j)(\{t, X\}_n) \leqslant \hat{f}_j$; use induction on j and replace the product on the right part of Eq. (10) by 1. Thus, for $|z| \leqslant 1/eC(\beta)$, the series (7) converges and Eq. (3) possesses a unique solution—compare with the consequence of Theorem 1 of ref. 7. Denote

$$\Psi_\beta(x) = \int |\chi_\beta(x+y) - \chi_\beta(y)| \, dy \leqslant 2C(\beta)$$

Lemma 4. There exist nonnegative values $C_{j,n} < +\infty$ such that

$$\begin{aligned} &|f_n(j)(\{1, x_1'\}, \{t_2, x_2\},..., \{t_{n-1}, x_{n-1}\}, \{1, x_n\}) \\ &\quad - f_n(j)(\{1, x_1''\},..., \{t_2, x_2\}, \{t_{n-1}, x_{n-1}\}, \{1, x_n\})| \\ &\leqslant C_{j,n} \Psi_\beta(x_1' - x_1'') \end{aligned}$$

Proof. We use induction (on j). Take $C_{1,n} = 1$ [see Eq. (8)]. Furthermore, one may take $C_{1,n} = 0$ for $n > N$ (see Lemma 1). We have

$$\begin{aligned} &|f_n(J+1)(\{1, x_1'\}, \{t_2, x_2\},..., \{t_{n-1}, x_{n-1}\}, \{1, x_n\}) \\ &\quad - f_n(J+1)(\{1, x_1''\},..., \{t_2, x_2\}, \{t_{n-1}, x_{n-1}\}, \{1, x_n\})| \\ &= \int_0^1 dt_n \int_{R^\nu} dy\, \chi_\beta(x_n - y) \prod_{l=\max(2, n-N+1)}^{n-1} [1 - t_l \chi_\beta(x_l - y)] \sum_{|\sum_{k=1, j(k)\geqslant 0}^{J} kj(k) = J|} \\ &\quad \times \Bigg| [1 - s\chi_\beta(x' - y)] \prod_{k=1}^{J} [f_{n+1}^{j(k)}(k)(\{1, x_1'\},..., \{1, y\})/j(k)!] \\ &\quad - [1 - s\chi_\beta(x'' - y)] \prod_{k=1}^{J} [f_{n+1}^{j(k)}(k)(\{1, x_1''\},..., \{1, y\})/j(k)! \Bigg| \end{aligned}$$

Here $s = 1$ if $n \leqslant N$ and $s = 0$ if $n > N$. One should:

(a) Replace the product

$$\prod_{l=\max(2, n-N+1)}^{n-1} [1 - t_l \chi_\beta(x_l - y)]$$

by 1.

(b) Add and substract (in brackets $|\cdots|$) the terms

$$\begin{aligned} &[1 - s\chi_\beta(x' - y)] \left[\prod_{k=1}^{J} f_{n+1}^{j'(k)}(k)(\{1, x_1'\},..., \{1, y\}) \right] \\ &\quad \times \prod_{k=1}^{J} [f_{n+1}^{j''(k)}(k)(\{1, x_1''\},..., \{1, y\})/j(k))!] \end{aligned}$$

and

$$\left[\prod_{k=1}^{J} f_{n+1}^{j'(k)}(k)(\{1, x_1'\},..., \{1, y\})\right]$$
$$\times [1 - s\chi_\beta(x'' - y)] \prod_{k=1}^{J} [f_{n+1}^{j''(k)}(k)(\{1, x_1''\},..., \{1, y\})/j(k)!]$$

for integer $j'(k) \geqslant 0$, $j''(k) \geqslant 0$, such that $j'(k) + j''(k) = j(k)$.

(c) Use the inequalities $f_n(j) \leqslant \hat{f}_j$ and conjecture that the statement is valid for $j = J$ in order to end the proof.

If the solution of Eq. (3) is unique [for example, for $zC(\beta) < e^{(4)}$], then the relation

$$H_{l+n}(\{0, Y\}_l, \{t, X\}_n) = H_n(\{t, X\}_n)$$

is valid for arbitrary natural n and l. We obtain

$$f_{l+n}(j)(\{0, Y\}_l, \{t, X\}_n) = f_n(j)(\{t, X\}_n)$$

having differentiated $\ln H_n$ by z. We use the notations $G_N^*(r^*) = G_N(x_1, x_2)$, and

$$G_{N,j}^*(r^*) \stackrel{\text{def}}{=} G_{N,j}(x_1, x_2)$$
$$\stackrel{\text{def}}{=} f_2(j)(\{0, x_1\}, \{1, x_2\}) - f_2(j)(\{1, x_1\}, \{1, x_2\}) \geqslant 0$$

for $r^* = |x_1 - x_2|/\sigma$. Thus

$$\ln G_N^*(r^*) = -\beta U(x_1 - x_2) - \sum_{j=1}^{+\infty} G_{N,j}^*(r^*)(-z)^j \tag{11}$$

$$\begin{aligned} G_{N,j}^*(r^*) &> 0 \quad \text{if} \quad r^* < \min(j+1, N) \quad \text{(see Lemma 3)} \\ &= 0 \quad \text{if} \quad r^* > \min(j+1, N) \quad \text{(see Lemma 2)} \end{aligned}$$

Proposition 1. Let

$$\lim_{x \to 0} \Psi_\beta(x) = 0 \tag{12}$$

Then one can find positive z_n for $n \leqslant N-2$ such that $G_N^*(r^*) - 1$ for r^* from $[1, n+1]$ changes its signature at least n times for any z from $[0, z_n]$. The roots of the equation $G_N^*(r^*) = 1$ for $z \downarrow 0$ converge to integer points j $(j = 2, n+1)$.

Proof. Relation (12) is a sufficient condition of continuity of $G^*_{N,j}(r^*)$ on r^* [see Lemma 4 and the definition of $G^*_{N,j}(r^*)$]. We have

$$\ln G^*_N(r^*) = -(-z)^j [G^*_{N,j}(r^*) - zG^*_{N,j+1}(r^*)] + O(z^{j+2})$$

for r^* from $[j, j+1]$, $1 \leqslant j \leqslant n \leqslant N-2$, because the first j items of the series (11) vanish for such values of r^*. This fact is used below without mention. If $z > 0$ is rather small, then

$$\operatorname{sign} \ln G^*_N(j) = -(-1)^j, \qquad \operatorname{sign} \ln G^*_N(j+1) = (-1)^j$$

and $\ln G^*_N$ changes its signature at least once for

$$r^* = r^*_{N,j}(z) \stackrel{\text{def}}{=} \inf\{r^* : j \leqslant r^* \leqslant j+1, \ln G^*_N(r^*) = 0\}$$

due to the Cauchy theorem. We have

$$G^*_{N,j}(r^*_{N,j}(z)) - zG^*_{N,j+1}(r^*_{N,j}(z)) = O(z^2) \qquad \text{for} \quad z > 0$$

The functions $G^*_{N,j}(r^*)$ are continuous and bounded. That is why

$$G^*_{N,j}(\inf \lim_{z \downarrow 0} r^*_j(z)) = 0 \Rightarrow \inf \lim_{z \downarrow 0} r^*_j(z) = j+1$$

[see properties of $G^*_{N,j}$ written out just below Eq. (11)]. Thus, all solutions r^* from $(j, j+1]$ of equations

$$\ln G^*(r^*) = 0 \Leftrightarrow G^*(r^*) = 1$$

converge to $j+1$ [see definition of $r^*_{N,j}(z)$].

One can find positive a, b, and z_n such that $|b| < 1$, $z_n < 1/eC(\beta)$,

$$\sup_{j \leqslant r \leqslant j+1} |\ln G^*_N(r)| = \sup_{j \leqslant r \leqslant j+1} \left| \sum_{k=j}^{+\infty} G^*_{N,k}(r)(-z)^j \right| < 2\hat{f}_j z_n^j < ab^j$$

and the series (11) oscillates for $z \leqslant z_n$ (use series for $\hat{f}$). One should use the expansion $e^x = 1 + x + O(x^2)$ in order to prove the same statement for the function $|G^*_N(r^*) - 1|$.

Activity increases iff density increases for small values of both of them $[d\rho(0)/dz = 1 > 0]$. The amplitudes of oscillations of $\ln G^*_N(r^*)$ and of $G^*_N(r^*) - 1$ being equal,

$$z^j \sup_{j \leqslant r \leqslant j+1} |G^*_{N,j}(r)| + O(z^{j+1}), \qquad j = 1, 2, ..., n-1$$

increases for rather small increasing values of density and activity. If we replace the product

$$\prod_{l=1}^{\max(0,n-N)} [1 - t_l \chi_\beta(x_l - y)]$$

by 1 in order to take into account only N particle interaction, we change the functions $G^*_{N,j}$, $j = N, N+1,\dots$, in such a way that the radial distribution function (approximated) $G^*_N(r^*)$ equals 1 for r^* from $[N, +\infty]$.

Proposition 2. $G^*_N(r^*)$ monotonically decreases (increases) for r^* from $(N-1, N)$ and even (odd) N if $U(x-y)$ is the pair repulsive potential with finite radius of interaction σ.

Proof. For $|x_1 - x_2| > \sigma$,

$$\begin{aligned} &H_2(\{1, x_1\}, \{1, x_2\}) \\ &\quad = \prod_{l=2}^{N} \exp\left\{ -z \int_0^1 dt_l \int_{R^\nu} dx_{l+1}\, \chi_\beta(x_l - x_{l+1}) \prod_{j=1}^{l-1} [1 - t_j \chi_\beta(x_j - x_{l+1})] \right. \\ &\qquad \left. \times H_{N+1}(\{t, X\}_{N+1}) \cdots \right\}, \qquad t_1 = t_{N+1} = 1 \end{aligned}$$

Here the product stands for a product of nonlinear operators and $H_{N+1}(\{t, X\}_{N+1})$ does not depend on $\{t, X\}_1$.[4] We can suppose $|x_l - x_{l+1}| \leqslant \sigma$ for $l = \overline{2, N}$. Thus, $|x_l - x_2| \leqslant (l-2)\sigma$ for $k = \overline{2, N+1}$. From the triangle inequality one obtains for $|x_1 - x_2| > (N-1)\sigma$

$$|x_1 - x_l| > (N - l + 1)\sigma \Rightarrow \chi_\beta(x_1 - x_l) = 0 \qquad \text{for} \quad l = \overline{3, N}$$

For

$$|x_1 - x_2| > (N-1)\sigma > |x_{N+1} - x_2|$$

the distance $|x_1 - x_{N+1}|$ increases with increasing $|x_1 - x_2|$.

3. GENERALIZED STRICT POSITIVITY AND PERRON–FROBENIUS THEOREM

Let us denote the space of functions defined on Γ_N, measurable and essentially bounded with respect to the measure

$$\prod_{k=1}^{N-1} (dt_k\, dx_k)\, [1 + \delta(t_N - 1)]\, dt_N\, dx_N$$

as B_N, its subset of continuous functions as C_N with a norm

$$|h| = \operatorname*{es\,sup}_{\{t,X\}_N \in \Gamma_N} |h(\{t, X\}_N)|$$

We define $f = f(h)$ from B_{N-1} for translation-invariant h from B_N,

$$f(\{t, X\}_{N-1}) = h\left(\left\{t_1, \sum_{l=1}^{N-1} x_l\right\}, \ldots, \left\{t_j, \sum_{l=j}^{N-1} x_l\right\}, \ldots, \{1, 0\}\right) \tag{13}$$

i.e., introduce new arguments—differences of coordinates—instead of coordinates in order to obtain a compact space of arguments. Define the action of the linear bounded operator P on B_{N-1} as

$$\begin{aligned} Pf(\{t, X\}_{N-1}) = \int_0^1 dt_N \int_{R^\nu} dx_N\, \chi_\beta(x_N) \prod_{l=1}^{N-1} \left[1 - t_l \chi_\beta\left(\sum_{k=l}^{N} x_k\right)\right] \\ \times f(\{t_2, x_2\}, \ldots, \{t_{N-1}, x_{N-1}\}, \{t_N, x_N\}) \end{aligned} \tag{14}$$

and the nonlinear operator S_N acting on B_N as follows

$$\begin{aligned} &S_N(h)(\{t, X\}_N) \\ &\quad = \exp\left\{-z \int_0^{t_N} dt'_N \int_{R^\nu} dy\, \chi_\beta(x_N - y) \prod_{l=1}^{N-1} [1 - t_l \chi_\beta(x_l - y)] \right. \\ &\qquad \left. \times h(\{t_2, x_2\}, \ldots, \{t'_N, x_N\}, \{1, y\})\right\} \end{aligned}$$

The equation[4] $h = S_N(S_N(h))$ is rewritten in terms of $f(h)$ as

$$f = \exp[-zP \exp(-zPf)] \tag{15}$$

[the value of $\exp(\cdots)$ is calculated at every point]. We suppose below $\operatorname{diam} \operatorname{supp} U = 2\sigma < +\infty$ and Eq. (12) to be valid. The solution f of Eq. (15) is determined by its values on

$$M_{N-1} = \{\{t, X\}_{N-1} \in \Gamma_{N-1} \colon |x_k| < \sigma,\ k = 1, N-1\}$$

It is a continuous function because of Eq. (12). Denote $w_1 = f$, $w_2 = \exp(-zPf)$; $B = [zw_1 Pzw_2 P]^{N-1}$ is a linear operator determined by the bounded (measurable) kernel $B(\{t, X\}_{N-1}, \{s, Y\}_{N-1})$ and measure

$$dm(\{s, Y\}_{N-1}) = \sum_{l=1}^{N-1} (ds_l\, dy_l)$$

zw_jP is the composition of P and the operator of multiplication (at every point of the arguments) by zw_j. One can prove that the value

$$\int_{R^\nu} |B(\{t', X'\}_{N-1}, \{s, Y\}_{N-1}) - B(\{t, X\}_{N-1}, \{s, Y\}_{N-1})| \, dm(\{s, \ Y\}_{N-1})$$

converges to zero uniformly for $\{t', X'\}_{N-1} \to \{t, X\}_{N-1}$ using Eq. (12) and performing some manipulations just as in the proof of Lemma 4. Thus B is a compact operator. Let us define

$$Q(v) = \inf_{Q \geqslant 0, Bv \leqslant Q|v| B1} Q, \qquad q(v) = \sup_{q \geqslant 0, Bv \geqslant q|v| B1} q \tag{16}$$

for any nonnegative function v from $C(M_{N-1})$: $Q(v) \leqslant 1$, $q(v) \geqslant 0$. Here and below we use the notation $B1$ for the image of the function that is equal to 1 at each point of M_{N-1}. Obviously $|Bv| \leqslant |v| \, |B1|$ for arbitrary v. One supposes that there exists a nonnegative vector 1 such that $Q(v) < +\infty$, $q(v) > 0$, for any v in order to generalize the results of the section to the case of abstract space.

Proposition 3. For arbitrary $v \geqslant 0$ from $C(M_{N-1}) \backslash \{0\}$,

$$q(v) > 0 \tag{17}$$

Proof. One can estimate $e^{-zC(\beta)} \leqslant w_j \leqslant 1$,

$$\begin{aligned} Bv(\{t, X\}_{N-1}) &\geqslant e^{-2(N-1)zC(\beta)} \\ &\quad \times \prod_{l=0}^{N-1} \left\{ z \int_0^1 du_l \int_{R^\nu} dw_l \, \chi_\beta(w_l) \prod_{j=1}^{l-1} (1 - u_j) \right. \\ &\quad \times \left. \prod_{j=l}^{N-1} \left[1 - t_j \chi_\beta \left(\sum_{k=j}^{N-1} x_k + \sum_{k=1}^{l} w_k \right) \right] \right\} \\ &\quad \times \prod_{l=1}^{N-1} \left\{ z \int_0^1 ds_l \int_{R^\nu} dy_l \, \chi_\beta(y_l) \prod_{j=l}^{N-1} (1 - u_j) \prod_{j=1}^{l-1} (1 - s_j) \right\} v(\{s, Y\}_{N-1}) \end{aligned}$$

Denoting

$$\begin{aligned} q &= e^{-2(N-1)zC(\beta)} z^{2(N-1)} |v|^{-1} [NC(\beta)]^{1-N} \\ &\quad \times \int_{M_{N-1}} \left\{ \prod_{l=1}^{N-1} (1 - s_l)^{N-l} \chi_\beta(y_l) \right\} v(\{s, Y\}_{N-1}) \, dm(\{s, y\}_{N-1}) > 0 \end{aligned}$$

we have $Bv \geqslant q|v| B1$.

Theorem 1. Let M_{N-1} be some compact set, and B be a linear nonnegative compact operator on $C(M_{N-1})$ satisfying inequality (17). Then the spectral radius of B is its eigenvalue with multiplicity equal to 1 with nonnegative eigenvector.

Proof. Define the function $r(v)$ for v from the cone of nonnegative functions $K^+ = C^+(M_{N-1})$ differing from zero: $r(v) = \sup_{r'v \leqslant Bv} r'$. We have

$$r(av) = r(v) \leqslant r(Bv)$$

for arbitrary $a > 0$. Let $\{v_j\}$ be a sequence of elements from $B\{y \in K^+ : |y| = 1\}$ such that

$$\lim_{J \to +\infty} r(v_j) = \sup r(v) = r$$

There exists a point of accumulation $v = \lim_{k \to \infty} v_{j(k)}$ with $r(v) = r \geqslant r(B1) \geqslant q(B1)$. If the equality

$$(B - r)v = 0 \tag{18}$$

is not valid, then the inequalities

$$B(B-r)v = BBv - rBv \geqslant q(Bv - rv)\,|Bv - rv|\,B1$$
$$\Rightarrow BBv \geqslant (r + q(Bv - rv)\,|Bv - rv|/|v|)\,Bv$$

contradict the definition of $r(v)$.

Each f from $C(M_{N-1})$ can be expanded in the following manner:

$$f = [f]_1 - [f]_2 + i([f]_3 - [f]_4)$$

for $[f]_1$, $[f]_2$, $[f]_3$, $[f]_4$ nonnegative (i.e., from K^+) such than (i) $[f]_1 - [f]_2$ and $[f]_3 - [f]_4$ are determined uniquely; and (ii) if $f = f_1 - f_2 + i(f_3 - f_4)$ for f_1, f_2, f_3, and f_4 from K^+, then $[f]_j \leqslant f_j$ for $j = 1, 2, 3, 4$.

$[f]_1$ is one-half of the sum of the absolute value of the real part of f and the real part of f, and $[f]_2$ is one-half of their difference; $[f]_3$ is one-half of the sum of the absolute value of the imaginary part of f and the imaginary part of f, and $[f]_4$ is one-half of their difference for f from $C(M_{N-1})$. Obviously,

$$[a([f]_1 - [f]_2 + i[f]_3 - i[f]_4)]_j = a[f]_j$$

for any positive real a and $j = 1, 2, 3, 4$. If $u = Bw$, then

$$[u]_1 - [u]_2 = B([w]_1 - [w]_2), \qquad [u]_3 - [u]_4 = B([w]_3 - [w]_4)$$

which means that the operator B is real.

Suppose that there exists $w = [w]_1 - [w]_2 + i([w]_3 - [w]_4)$ being an eigenvector of B with eigenvalue $a = |a| e^{i\phi}$: $Bw = aw$, such that $|a| > r$. Then

$$\begin{aligned}
&-Q([w]_1 + [w]_2) \, |[w]_1 + [w]_2| \, Bv/q(v) \, |v| \\
&\quad \leqslant -Q([w]_1 + [w]_2) \, |[w]_1 + [w]_2| \, B1 \\
&\quad \leqslant -B([w]_1 + [w]_2) \\
&\quad \leqslant B([w]_1 - [w]_2) \\
&\quad \leqslant B([w]_1 + [w]_2) \\
&\quad \leqslant Q([w]_1 + [w]_2) \, |[w]_1 + [w]_2| \, B1 \\
&\quad \leqslant Q([w]_1 + [w]_2) \, |[w]_1 + [w]_2| \, Bv/q(c) \, |v|
\end{aligned}$$

and

$$\begin{aligned}
&-Q([w]_3 + [w]_4) \, |[w]_3 + [w]_4| \, Bv/q(v) \, |v| \\
&\quad \leqslant -Q([w]_3 + [w]_4) \, |[w]_3 + [w]_4| \, B1 \\
&\quad \leqslant -B([w]_3 + [w]_4) \\
&\quad \leqslant B([w]_3 - [w]_4) \\
&\quad \leqslant B([w]_3 + [w]_4) \\
&\quad \leqslant Q([w]_3 + [w]_4) \, |[w]_3 + [w]_4| \, B1 \\
&\quad \leqslant Q([w]_3 + [w]_4) \, |[w]_3 + [w]_4| \, Bv/q(v) \, |v|
\end{aligned}$$

[see definition (16)]. That is why

$$\begin{aligned}
B([w]_1 - [w]_2 + c_1 v) &\geqslant 0 \\
B([w]_2 - [w]_1 + c_2 v) &\geqslant 0 \\
B([w]_3 - [w]_4 + c_3 v) &\geqslant 0 \\
B([w]_4 - [w]_3 + c_4 v) &\geqslant 0
\end{aligned}$$

for

$$\begin{aligned}
c_1 = c_2 &= Q([w]_1 + [w]_2) \, |[w]_1 + [w]_2| / |v| \, q(v) \\
c_3 = c_4 &= Q([w]_3 + [w]_4) \, |[w]_3 + [w]_4| / |v| \, q(v)
\end{aligned}$$

Let $1<n_1<n_2<n_3<\cdots$ be a sequence of natural numbers such that $\exp(in_k\phi)\to 1$ while $k\to +\infty$. Obviously,

$$|a|^{-nk}B^{nk}([w]_1-[w]_2+c_1v)\geqslant 0$$

$$|a|^{-nk}B^{nk}([w]_2-[w]_1+c_2v)\geqslant 0$$

$$|a|^{-nk}B^{nk}([w]_3-[w]_4+c_3v)\geqslant 0$$

$$|a|^{-nk}B^{nk}([w]_4-[w]_3+c_4v)\geqslant 0$$

We obtain $[w]_1\leqslant[w]_2\leqslant[w]_1$ and $[w]_3\leqslant[w]_4\leqslant[w]_3$, having used the following equalities:

$$|a|^{-nk}B^{nk}([w]_1-[w]_2+i([w]_3-[w]_4))=|a|^{-nk}B^{nk}w=e^{ink\phi}w\to w$$

$$|a|^{-nk}B^{nk}c_jv=c_j(r/|a|)^{nk}v\to 0 \qquad \text{while} \quad k\to +\infty$$

This implies $[w]_1=[w]_2$, $[w]_3=[w]_4\Rightarrow w=0$, i.e., our supposition was invalid, i.e., the absolute value of any eigenvalue of B is not greater than r, i.e., r is the spectral radius of B.

Let w be any element from $\ker(B-r)\backslash\{0\}$. Then $B([w]_1-[w]_2)=r([w]_1-[w]_2)$, $B([w]_3-[w]_4)=r([w]_3-[w]_4)$, the operator B is real. We obtain $B[w]_j\geqslant r[w]_j$ $(j=1, 2, 3, 4)$ applying $[\cdot]_1$ and $[\cdot]_2$ to the latest equalities and using property (ii). Thus, $[w]_j$ $(j=1, 2, 3, 4)$ satisfies Eq. (18)—see the definition of r. That is why it is enough to prove that any u from $K^+\cap\ker(B-r(B))\backslash\{0\}$ coincides with v up to some nonnegative multiplier in order to prove that $\dim\ker(B-r)=1$. Define

$$a=\sup_{u\geqslant bv} b\leqslant Q(u)\,|u|/q(v)\,|v|$$

If u does not equal av,

$$\begin{aligned} u-av=B(u-av)/r &\geqslant q(u-av)\,|u-av|\,B1/r \\ &\geqslant q(u-av)\,|u-av|\,v/Q(v)\,|v| \end{aligned}$$

which contradicts the definition of a.

Note that the theorem is proved for an operator B that is not strictly positive, i.e., we generalize Theorem 6.3 of ref. 11 for the case of abstract space (not only the space of functions) and not strictly positive operator B, supposing the existence of the expansion $w=[w]_1-[w]_2+i([w]_3-[w]_4)$ with properties (i)–(ii) and the existence of a nonnegative vector 1 such that $Q(w)<\infty$ and $q(w)>0$ for any nonnegative w.

We use the notation $r(B)$ for the spectral radius of operator B. Define

$$M'_{N-1}=\{\{t, X\}_{N-1}: 0\leqslant t_j<1, 0\leqslant |x_j|\leqslant\sigma\}$$

Taking positive

$$q=\int df^*(\{t, X\}_{N-1}) \prod_{l=1}^{N-1} (1-t_l)^l e^{-2(N-1)zC(\beta)} z^{2(N-1)}/m(M_{N-1})N^{N-1}$$

for $f^* \geqslant 0$ from $C^*(M_{N-1})$, $f^*(M'_{N-1})>0$, one can estimate the Radon–Nikodym derivative

$$dB^*f^*(\{t, X\}_{N-1})/dm > q\ dB^*m(\{t, X\}_{N-1})/dm \tag{19}$$

The right part of the inequality is positive on M'_{N-1}; thus, the solution of the equation $[B^*-r(B)]f^*=0$ can be taken positive on M'_{N-1}. The solution of Eq. (18) should be taken positive on M'_{N-1} also. We have

$$\dim\ker[B^*-r(B)]=\dim\ker[B-r(B)]=1 \tag{20}$$

Let V be a Banach space, and A be an endomorphism of V such that A^k is compact for some natural k; then the Fredholm alternative is valid for $1-A$.[12] If the statement of Theorem 1 is valid for $B=A^k$, then it is valid for $B=A$.

4. BIFURCATION OF THE SOLUTIONS OF THE APPROXIMATE EQUATION OF STATE

Denote the solution of the equation $f=e^{-zPf}$ as $f(z)$,

$$z_0=\sup\{z'>0: z<z' \Rightarrow r(zf(z)P)<1\}$$

We suppose z_0 to the finite, otherwise Eq. (15) has only one solution for any $z>0$. There exists a point of accumulation of the equibounded and equicontinuous functions

$$f_0=\lim_{z_k \uparrow z_0} f(z_k), \qquad f_0=\exp(-z_0 Pf_0)$$

$r(z_0 f(z_0)p)=1$; otherwise, there is a contradiction with the definition of z_0. The $(1+z_0 f_0 P)^{-1}$ does not exist (as bounded operator) iff -1 is an eigenvalue of $z_0 f_0 P$ (see the last paragraph of Section 3). This condition implies $\dim\ker(1-B)\geqslant 2$ for $B=(z_0 f_0 P)^{2(N-1)}$, which contradicts Theorem 1. Thus, there exists a bounded linear operator $(1+z_0 f_0 P)^{-1}$ and $f(z)$ can be prolonged smoothly for $z>z_0$:

$$df(z_0)/dz= -(1+z_0 f_0 P)^{-1} f_0 P f_0$$

Denote the pair of real numbers $Z=(z, z^*)$ and define the nonlinear operators S, F, and G acting on $C(M_{N-1})$,

$$S(f, Z)=\exp(-zPf)$$

$$F(f, Z)=\exp(-z\langle f^*f\rangle\, Pf)$$

$$G(f, Z)=S(F(f, Z), Z)$$

where

$$f^*\in\ker[1-L^*(z_0)]\backslash\{0\}, \qquad L(z)=zf(z)P \tag{21}$$

and $\langle f^*f\rangle$ is the value of the functional f^* on the vector f. Here the symbols F and G denote objects other than in Sections 1–3. Take

$$z_0^*=z_0/\langle f^*f_0\rangle, \qquad Z_0=(z_0, z_0^*) \tag{22}$$

Below we distinguish below $PvPw$—the result of action of P on the product of v and Pw—and $(Pv)(Pw)$, which is the product of Pv and Pw. Sometimes we do not indicate the dependence of functions and operators on f and Z.

Lemma 5. There exists a bounded operator $(1-\partial G(f_0, Z_0)/\partial f)^{-1}$.

Proof. We have

$$\partial G(f_0, Z_0)/\partial f=L^2(z_0)+f_1(f_0, Z_0)\rangle\langle f^*$$

where

$$f_1(f, Z)=zGPz^*FPf, \qquad \langle f^*f_1(f_0, Z_0)\rangle=1$$

and $v\rangle\langle f^*$ is a one-dimensional operator, acting as follows:

$$[v\rangle\langle f^*]h=\langle f^*h\rangle v$$

The operator

$$(L^2+f_1\rangle\langle f^*)^{N-1}$$

is a compact one as the sum of compact $B=L^{2(N-1)}$ and the sum of $2^{N-1}-1$ one-dimensional operators. Thus, the Fredholm alternative is valid for $1-L^2-f_1\rangle\langle f^*$. The equation

$$[1-L^2(z_0)]\,w=\langle f^*w\rangle\, f_1(f_0, Z_0)$$

possesses a solution w iff $\langle f^*w\rangle\langle f^*f_1\rangle = 0$, which implies that w is from $\ker(1 - L(z_0))$ and $\langle f_0^*w\rangle = 0$, implying $w = 0$ because of the signature constancy of the elements of $\ker(1 - L(z_0))$ and $\ker(1 - L(z_0)^*)$.

Denoting the analytic functions $R(z) = r(L(z))$ and $v(z)$ from $\ker[R(z) - L(z)]$, we obtain

$$dR/dz = \langle v^*(dL/dz)v\rangle/\langle v^*v\rangle$$

from

$$(dR/dz - dL/dz)v + (R - L)\,dv/dz = 0$$

Below we suppose the following condition to be valid:

$$dR(z_0)/dz = \langle f^*v(z_0)\{[1 + L(z_0)]^{-1}f_0\}/z_0f_0\rangle/\langle f^*v(z_0)\rangle > 0 \quad (23)$$

The equation

$$f = G(f, Z) \quad (24)$$

possesses a unique solution for Z from the neighborhood of Z_0. Denote this solution as $f(Z)$ and set $\phi(Z) = z - z^*\langle f^*f(Z)\rangle$.

$$\phi(Z) = 0 \Leftrightarrow f(Z) = \exp\{-zP\exp[-zPf(Z)]\} \quad (25)$$

Theorem 2. If conditions (21)–(23) are valid, then

$$d\phi(Z_0) = 0, \qquad d^2\phi(Z_0) = [dR(z_0)/dz][3dz - 2(z_0/z_0^*)\,dz^*]\,dz$$

i.e., Z_0 is a hyperbolic-type singular point of the curve (25).

Proof. We have

$$d\phi = (1 - z^*\langle f^*\partial f/\partial z\rangle)\,dz - (\langle f^*f\rangle + z^*\langle f^*\partial f/\partial z^*\rangle)\,dz^*$$

Having differentiated Eq. (24) for $Z = Z_0$, we obtain

$$[1 - L^2(z_0)]\,\partial f(Z_0)/\partial z = \langle f^*\,\partial f(Z_0)/\partial z\rangle f_1(f_0, Z_0) + \partial G(f_0, Z_0)/\partial z \quad (26)$$

$$[1 - L^2(z_0)]\,\partial f(Z_0)/\partial z^* = \langle f^*\,\partial f(Z_0)/\partial z^*\rangle\, f_1(f_0, Z_0) + \partial G(f_0, Z_0)/\partial z^* \quad (27)$$

where $\partial G/\partial z = -(GPF)$, $\partial G/\partial z^* = (zGP\langle f^*f\rangle FPf)$. The Fredholm alternative gives

$$\langle f^* \,\partial f(Z_0)/\partial z^*\rangle = -\langle f^*f_0\rangle/z_0^* \tag{28}$$

$$\Rightarrow \partial f(Z_0)/\partial z^* \in \ker[1 - L(z_0)] \tag{29}$$

$$\langle f^* \,\partial f(Z_0)/\partial z\rangle = \langle f^*f_0\rangle/z_0 \tag{30}$$

$$\Rightarrow \partial f(Z_0)/\partial z = -L(z_0)[1 + L(z_0)]^{-1} f_0/z_0 - (3z_0^*/2z_0)\,\partial f(Z_0)/\partial z^* \tag{31}$$

Indeed, Eq. (26) at the point

$$(f, Z) = (f_0, Z_0) \tag{32}$$

for (30) takes form

$$(1 - L^2)\,\partial f/\partial z = -L(1 - L) f/z$$

Thus, $\partial f(Z_0)/\partial z$ can be represented as follows:

$$\partial f(Z_0)/\partial z = -L(z_0)[1 + L(z_0)]^{-1} f_0/z_0 + a\,\partial f(Z_0)/\partial z^*$$

where the constant a is determined uniquely from Eq. (30). Thus, $d\phi(Z_0) = 0$.

We suppose equality (32) to be valid below in the calculation of the value of the corresponding derivatives, which implies

$$\langle f^* zfPv\rangle = \langle f^*v\rangle, \qquad zfP\,\partial f/\partial z^* = \partial f/\partial z^*$$

Denoting $A = zGPz^*\langle f^*f\rangle FP$, we obtain

$$\begin{aligned}(1 - A)\,\partial^2 f/\partial z^{*2} = {}& \langle f^*\,\partial^2 f/\partial z^{*2}\rangle f_1 + \partial^2 G/\partial z^{*2} \\ & + 2(\partial^2 G/\partial z^*\,\partial f)\,\partial f/\partial z^* \\ & + (\partial^2 G/\partial f^2)(\partial f/\partial z^*, \partial f/\partial z^*)\end{aligned} \tag{33}$$

having differentiated (24), where

$$\partial^2 G/\partial z^{*2} = (Af/z^*)^2/G - zGPF(\langle f^*f\rangle Pf)^2 \tag{34}$$

$$\begin{aligned}(\partial^2 G/\partial z^*\,\partial f)v = {}& (Af/z^*)[(\partial G/\partial f)v]/G + (\partial G/\partial f)v/z^* \\ & - zGPF(\langle f^*f\rangle Pf)(z^*\langle f^*f\rangle Pv + z^*\langle f^*v\rangle Pf)\end{aligned} \tag{35}$$

$$\begin{aligned}(\partial^2 G/\partial f^2)(v, w) = {}& [(\partial G/\partial f)v][(\partial G/\partial f)w]/G \\ & + (\langle f^*v\rangle Aw + \langle f^*w\rangle Av)/\langle f^*f\rangle \\ & - zGPz^{*2}F(\langle f^*f\rangle Pv + \langle f^*v\rangle Pf) \\ & \times (\langle f^*f\rangle Pw + \langle f^*w\rangle Pf)\end{aligned} \tag{36}$$

Having substituted (28)–(29) and (34)–(36) in (33), we obtain

$$\langle f^* \, \partial^2 f(Z_0)/\partial z^{*2} \rangle = 2\langle f^* f_0 \rangle / z_0^{*2} \tag{37}$$

using the Fredholm alternative for (33). Obviously,

$$\partial^2 \phi/\partial z^{*2} = -2\langle f^* \, \partial f/\partial z^* \rangle - z^* \langle f^* \, \partial^2 f/\partial z^{*2} \rangle$$

which vanishes for (32). By analogy with (33),

$$\begin{aligned}(1-A)\, \partial^2 f/\partial z^2 = \langle f^* \, \partial^2 f/\partial z^2 \rangle f_1 + \partial^2 G/\partial z^2 \\ + 2(\partial^2 G/\partial z \, \partial f)\, \partial f/\partial z \\ + (\partial^2 G/\partial f^2)(\partial f/\partial z, \partial f/\partial z)\end{aligned} \tag{38}$$

$$\partial^2 G/\partial z^2 = G(PF)(PF) \tag{39}$$

$$(\partial^2 G/\partial z \, \partial f)\, v = (1/z - PF)[(\partial G/\partial f)\, v] \tag{40}$$

$$\partial^2 \phi/\partial z^2 = -z^* \langle f^* \, \partial^2 f/\partial z^2 \rangle \tag{41}$$

Having substituted (30)–(31), (36), (39), and (40) in (38), we obtain

$$\partial^2 \phi(Z_0)/\partial z^2 = -6 \, dR(z_0)/dz$$

using the Fredholm alternative for (38).

It is easy to prove the following equalities:

$$\begin{aligned}\partial^2 \phi(Z_0)/\partial z \, \partial z^* &= -(z_0/z_0^*)\, \partial^2 \phi(Z_0)/\partial z^2 \\ &= -2\langle f^* f_0 \rangle \, dR(z_0)/dz\end{aligned}$$

acting on (24) and (25) by $\partial^2/\partial z \, \partial z^*$ and using the Fredholm alternative in the manner demonstrated above in order to end the proof.[13]

If $dR(z_0)/dz = 0$, it is necessary to investigate $d^3\phi(Z_0)$. For the branch

$$dz(Z_0)/dz^* = 0 \tag{42}$$

$$d\rho(Z_0)/dz^* = z_0 \, \partial f(\{0, 0\}, ..., \{0, 0\})/\partial z^* \neq 0 \tag{43}$$

Note that the formulas (42)–(43) are in good qualitative agreement with Monte Carlo and molecullar dynamics simulations (see Fig. 2 of ref. 14). One should take large N in order to obtain a good quantitative agreement. We note that the singularity on activity appears before the singularity on density for $N = 2$.[10]

5. DECISION PROBLEM OF EQUATION $f=S_N(f)$

Theorem 3. There exists at least one solution of the equation

$$f=S_N(f)$$

for all positive values of z, if condition (12) is valid.

Proof. Let $\{a_n(t)\geqslant 0\}$, $\{b_n(t)\geqslant 0\}$ be sequences of functions converging to Dirac delta functions, defined on $[0, 1]$ and R^ν, respectively:

$$\text{diam supp } a_n = \text{diam supp } b_n < 1/n$$

$c_n(x)\geqslant 0$ is an infinitely differentiable function on R^ν:

$$c_n(x)\begin{cases} =1 & |x|\leqslant n \\ <1 & n<|x|<(n+1) \\ =0 & |x|\geqslant (n+1)\end{cases}$$

Let us consider the sequence of operators

$$\begin{aligned} &S_{N,n}(f)(\{t, X\}_N) \\ &\quad =\prod_{j=1}^{N} c_n(x_j) \\ &\qquad \times \exp\left\{-z\int_0^{t_N} dt'_N \int_{R^\nu} dy\, \chi_\beta(x_N-y) \prod_{j=1}^{N-1}[1-t_j\chi_\beta(x_j-y)]\right. \\ &\qquad \times \prod_{j=2}^{N-1}\int_0^1 dt'_j\, a_n(t'_j-t_j) \prod_{j=1}^{N-1}\int_{R^\nu} dx'_j\, b_n(x'_j-x_j) \\ &\qquad \left.\times f(\{t'_2, x'_2\},..., \{t'_N, x'_N\}, \{1, y\})\right\} \end{aligned}$$

Denote the Banach space of continuous functions, defined on Γ_N and vanishing at infinity (for spatial arguments), with a norm

$$\|f\| = \sup |f(\{t, X\}_N)|$$

as $C_0(\Gamma_N)$. Let

$$B=\{f\in C_0(\Gamma_N)\colon 0\leqslant f(\{t, X\}_N)\leqslant 1\}$$

be a closed, convex, bounded set, which is mapped into itself by the operator $S_{N,n}$ to be compact if condition (12) is calid. There is a fixed point

$$f^{(n)}(\{t, X\}_N)=S_{N,n}(f^{(n)}(\{t, X\}_N)) \qquad (44)$$

due to Shauder's theorem. The further proof is based on the fact that the operator $S^N_{N,n}(f)$ is compact (uniformly in n) in the topology of uniform convergence on each compact subset of Γ_N. We define

$$C_r = \{\{t, X\}_N \in \Gamma_N : |\{t, X\}_N| \leqslant r\}$$

where $|\cdot|$ is the Euclidian distance in Γ_N. One can prove that there exists n_0 (depending on r) and C (depending on N, $\|f\|$, and n_0) such that for $n > n_0$,

$$|S^N_{N,n}(f)(\{t, X\}_N) - S^N_{N,n}(f)(\{t, X\}'_N)| \leqslant C(N, \|f\|, n_0) \sum_{j=1}^{N} [|t_j - t'_j| + \Psi_\beta(x_j - x'_j)]$$

for $\{t, X\}_N$ and $\{t, X\}'_N$ from C_r. Because of the equality

$$f^{(n)}(\{t, X\}_N) = S^N_{N,n}(f^{(n)}(\{t, X\}_N)$$

and $\|f^{(n)}(\{t, X\}_N)\| \leqslant 1$, one can obtain

$$|f^{(n)}(\{t, X\}_N) - f^{(n)}(\{t, X\}'_N)| \leqslant C(N, 1, n_0) \sum_{j=1}^{N} [|t_j - t'_j| + \Psi_\beta(x_j - x'_j)]$$

i.e., the sequence $f^{(n)}(\{t, X\}_N)$ has an accumulation point due to Arzela's theorem. One can perform a limit transition in Eq. (44), because the accumulating point of the sequence $f^{(n)}_N(\{t, X\})$ is a continuous function whose values are in the segment [0, 1]. The theorem has been proved.

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